TRX AND UO2 CRITICALITY BENCHMARKS WITH SAM-CE

M. Beer, E. S. Troubetzkoy, H. Lichtenstein
Mathematical Applications Group, Inc.
3 Westchester Plaza
Elmsford, New York 10523

P. F. Rose
Brookhaven National Laboratory
Upton, New York 11973

ABSTRACT

A set of thermal reactor benchmark calculations with SAM-CE which have been conducted at both MAGI and at BNL are described. Their purpose was both validation of the SAM-CE reactor eigenvalue capability developed by MAGI and a substantial contribution to the data testing of both ENDF/B-IV and ENDF/B-V libraries. This experience also resulted in increased calculational efficiency of the code and an example is given.

The benchmark analysis included the TRX-1 infinite cell using both ENDF/B-IV and ENDF/B-V cross section sets and calculations using ENDF/B-IV of the TRX-1 full core and TRX-2 cell. BAPL-UO2-1 calculations were conducted for the cell using both ENDF/B-IV and ENDF/B-V and for the full core with ENDF/B-V. In these calculations the modeling of the full core lattices was accomplished by use of Complex Combinatorial Geometry. Eigenvalues, reaction rates and reaction rate ratios are given for these cases and the results discussed.

1. INTRODUCTION

This paper describes a set of Monte Carlo calculations with SAM-CE involving thermal reactor benchmarks. The calculations were performed recently at MAGI and at Brookhaven National Laboratory (BNL). They involved both full core and infinite cell cases, utilizing both the ENDF/B-IV and the ENDF/B-V libraries.

The dual major purpose of the calculations was the validation of the SAM-CE reactor capabilities that are described in other papers at this session and a contribution to the testing of data pertaining to reactors in the ENDF/B libraries.

Efforts were also made to utilize the experience gained in running problems with SAM-CE to improve the overall efficiency of the Monte Carlo calculations.

It is useful to briefly mention one example of improved efficiency before turning to the major considerations of this paper - the calculations and results. We refer to variance reduction by application of a posteriori statistical methods to several estimators of the same parameter. In particular, SAM-CE estimates k_{eff} in four ways, utilizing track length and collision type estimators. In the course of these calculations, the maximum likelihood-minimum variance procedure was first applied to the case of several eigenvalue estimators[1] and later implemented within SAM-CE directly[2]. The method was also applied to the case of two estimators of the same reaction rate in some of the later benchmark calculations.

2. CALCULATIONS AND METHODOLOGY

We now turn to consideration of the calculations. These involved the TRX-1, TRX-2 and BAPL-UO2-1 benchmarks. Results were obtained for the cases shown in Table 1. Note that calculations of TRX-1 and TRX-2 cells and the TRX-1 full core were conducted utilizing an available SAM-X processed library of ENDF/B-IV elements[3]. These calculations proved very useful in the code validation.

The BAPL-UO2-1 calculations for the cell were performed with both the ENDF/B-IV library and a recently processed ENDF/B-V SAM-CE library[4]. A full core ENDF/B-V calculation has also been performed. These SAM-CE benchmarks offered useful comparison of results involving both ENDF/B-IV and ENDF/B-V.

It should be noted that calculations involving the ENDF/B-V library utilize the fission spectra specified for the individual isotopes by ENDF/B-V at a particular neutron energy. The ENDF/B-IV calculations assumed fission spectra to be represented by that for ^{235}U thermal neutrons.

Geometry and composition for the problems are as specified in the "CSEWG Benchmark Specifications"[5]. Reflective boundary conditions were used for the cell combinatorial geometry. Full core calculations utilized complex combinatorial geometry.

All the benchmarks were run on CDC 7600 computers. The BAPL-UO2-1 ENDF/B-V benchmark was also run on a PDP-10 computer*. The BAPL-UO2-1 full core calculation was conducted at MAGI, the remainder at BNL.

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*The results given herein for this benchmark are those obtained on the PDP-10.

TABLE 1

Benchmark Criticality Calculations
Conducted with SAM-CE

Benchmark	Cell Calculation		Full Core	
	ENDF/B-IV	ENDF/B-V	ENDF/B-IV	ENDF/B-V
TRX-1	Yes	No	Yes	No
TRX-2	Yes	No	No	No
BAPL-UO2-1	Yes	Yes	No	Yes

3. RESULTS

The TRX-1 and TRX-2 cell eigenvalue and reaction rate ratios are given in Table 2 for SAM-CE calculations as well as comparison results obtained from the RECAP and VIM Monte Carlo codes*. Generally good agreement is found between the codes. Table 3 gives 4 group** reaction rates for ^{235}U and ^{238}U obtained for both the TRX-1 and TRX-2 cells.

We now turn to the TRX-1 full core results. Table 4 gives k_{eff} and inner core reaction rate ratios for SAM-CE and comparison BNL results for RECAP[6] and Hardy's RCP01 results[7]. The SAM-CE inner core was chosen to conform to the largest region shown by Hardy[7] to yield reaction rate ratios imperceptibly different from core center results.

The important deviations of calculated and experimental values occur for k_{eff} and ρ_{28} for which all three codes agree fairly well with each other. The effect is better seen in Figure 1 in which the SAM-CE and RECAP points have been added to the other points plotted previously by Hardy[6]. The deviations of k_{eff} and ρ_{28} from experiment clearly are artifacts of the ENDF/B-IV data.

The BAPL-UO2-1 calculations allow comparisons to be made between ENDF/B-IV and ENDF/B-V results. Table 5 contains values for k_{eff} and reaction rate ratios for the 3 cases considered. (Inner core reaction rates are given for the full core results.) Note first the good agreement obtained between the full core ENDF/B-V values and experiment. On the other hand, comparison of the cell results indicates a seemingly significant increase in the k_{eff} value from ENDF/B-IV to ENDF/B-V ($\sim$.6%) in conformity with the TRX results (low k_{eff} for ENDF/B-IV full core).

Turning to the reaction rates, Table 6 gives reaction rates for ENDF/B-IV and ENDF/B-V cell calculations in the CSEWG group structure. The significant changes in this case involve a decrease in ^{238}U fast capture and an increase in fast ^{238}U fission from ENDF/B-IV to ENDF/B-V. Reaction rates for ENDF/B-V results were also obtained in a second four group structure specified by EPRI***. These were divided by the group fluxes to obtain the EPRI group cross sections given in Table 7 for ENDF/B-V cell and full core calculations. Good agreement is obtained between full core inner core and cell results for all cases.

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*Uncertainties in all the tables are either standard deviations or percent standard deviations when indicated.

**Upper energy boundaries of the four groups are 10 MeV, 67.379 keV, 3.355 keV, 0.625 eV. These will be referred to as the CSEWG group structure.

***Upper energy boundaries of the four groups are 10 MeV, 821 keV, 5.53 keV and 0.625 eV.

TABLE 2

Eigenvalues and Reaction Rate Ratios
for TRX-1 and TRX-2 Cell Calculations

LATTICE PARAMETERS	TRX-1 RECAP	TRX-1 SAM-CE	TRX-1 VIM	TRX-2 RECAP	TRX-2 SAM-CE	TRX-2 VIM
k_∞	1.1721 ± .0019	1.1751 ± .0016	1.1721 ± .0030	1.1578 ± .0026	1.1605 ± .0015	1.1613 ± .0032
ρ_{28}	1.334 ± .46%	1.324 ± .8%	1.328 ±1.2%	.8244 ± .75%	.8139 ±1.1%	.8344 ±1.0%
δ_{25}	.0963 ± .52%	.09526± .7%	.09693± .87%	.05843± .82%	.0585 ± .9%	.05917± .86%
δ_{28}	.08903± .56%	.09206± .7%	.08866± .81%	.06473± .80%	.06450± .7%	.06487± .75%
C*	.7910 ± .31%	.7882 ± .4%	.7899 ± .78%	.6351 ± .43%	.6314 ± .5%	.6391 ± .58%

TABLE 3

CSEWG 4 Group Reaction Rates for TRX-1 and TRX-2 Cells
For ENDF/B-IV

Group	U-235 Capture	U-235 Fission	U-235 Neutron Production	U-238 Capture	U-238 Fission	U-238 Neutron Production
			TRX-1 Cell SAM-CE			
1	4.059-4 (.4%)	3.3806-3 (.3%)	8.8013-3 (.3%)	1.9124-2 (.3%)	4.0174-2 (.6%)	.11312
2	5.8811-4 (.7%)	1.5780-3 (.7%)	3.8208-3 (.7%)	2.3463-2 (.7%)	3.0653-7 (1.4%)	7.1361-7 (1.4%)
3	1.5904-2 (.9%)	.032998 (.6%)	7.9818-2 (.6%)	.15338 (.8%)	0	0
4	6.8756-2 (.4%)	.39846 (.4%)	.96381 (.4%)	.14799 (.4%)	0	0
			TRX-2 Cell SAM-CE			
1	2.5792-4 (.5%)	2.2535-3 (.4%)	5.8910-3 (.4%)	1.2370-2 (.5%)	2.8790-2 (.6%)	8.1126-2 (.6%)
2	3.5808-4 (.9%)	9.5908-4 (.9%)	2.3221-3 (.8%)	1.4222-2 (1.0%)	1.7960-7 (.23%)	4.1812-7 (2.3%)
3	1.0504-2 (1.2%)	2.1486-2 (.8%)	5.1973-2 (.8%)	9.9864-2 (1.1%)	0	0
4	7.2275-2 (.4%)	.42167 (.4%)	1.0199 (.4%)	.15537 (.4%)	0	0

TABLE 4

TRX-1 Full Core k_{eff} and Reaction Rate Ratios
For the Inner Core Region

PARAMETER	EXPERIMENT	RCPO1	RECAP	SAM-CE
k_{eff}	1	.9837 ± .0008	.9827 ± .0013	.9839 ± .0026
ρ_{28}	1.320 ± .021	1.396 ± .004	1.415 ± .021	1.390 ± .018
δ_{25}	.0987 ± .0010	.1009 ± .0005	.1015 ± .0016	.09989 ± .0013
δ_{28}	.0946 ± .0041	.0972 ± .0003	.09707 ± .0016	.09939 ± .0012
C*	.797 ± .008	.809 ± .001	.8167 ± .0095	.8070 ± .0056

TABLE 5

BAPL-UO2-1 Values for k_{eff} and Reaction Rate Ratios for FNDF/B-IV and ENDF/B-V Data

Parameters	Cell ENDF/B-IV	Cell ENDF/B-V	Full Core ENDF/B-V	Experiment
k	1.137 ± .0017	1 1433 ± .0019	0.9958 ± .0032	1
ρ_{28}	1.385 ± .011	1.392 ± .011	1.429 ± .062	1.39 ± .01
δ_{25}	0.0801 ± .0006	0.0806 ± .0005	0 0801 ± .0024	0.084 ± .002
δ_{28}	0.0710 ± .0004	0.0727 ± .0006	0.0764 ± .0027	0.078 ± .004
C*	0.8022 ± .0041	0.8058 ± .0038	0 819 ± .020	--

TABLE 6

BAPL-UO2-1 ENDF/B-IV and ENDF/B-V CSEWG Four Group Cell Reaction Rates

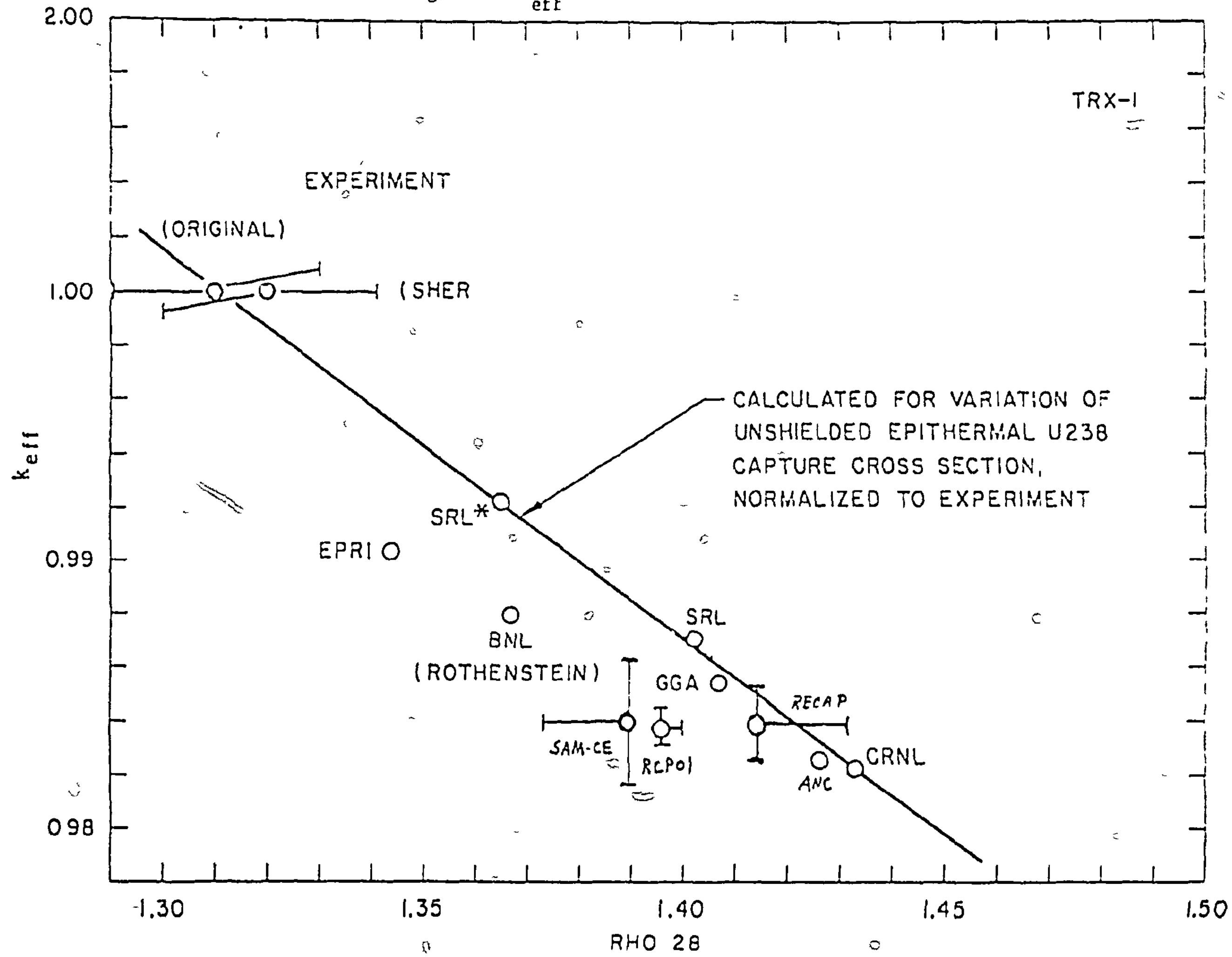
	ENDF/B-IV				ENDF/B-V PDP-10			
	^{235}U		^{238}U		^{235}U		^{238}U	
Group	Capture	Fission	Capture	Fission	Capture	Fission	Capture	Fission
1	3.186-4 (.34%)	2.628-3 (.30%)	1.467-2 (.32%)	3.086-2 (.48%)	3.177-4 (.37%)	2.643-3 (.35%)	1.430-2 (.37%)	3.1410-2 (.71%)
2	4.946-4 (.57%)	1.322-3 (.57%)	2.024-2 (.66%)	<1.-6	5.000-4 (.55%)	1.312-3 (.58%)	1.996-2 (.75%)	<1.-6
3	1.394-2 (.74%)	2.825-2 (.61%)	.1672 (.73%)	0	1.421-2 (.83%)	2.831-2 (.71%)	.16841 (.42%)	2.152-6 (12%)
4	6.932-2 (.36%)	.4027 (.36%)	.1463 (.35%)	0	6.895-2 (.25%)	.4003 (.25%)	.1457 (.25%)	0

TABLE 7

EPRI Four Group Cross Sections (barns) for BAPL-UO2-1 Cell and Full Core Using the ENDF/B-V Library

		Cell	Full Core (Inner)	Full Core - Cell
U235 Absorption	σ_1	1.2920 ± .0010	--	--
	σ_2	2.0750 ± .0039	--	--
	σ_3	38.478 ± .233	--	--
	σ_4	453.76 ± 1.47	--	--
U235 Fission	σ_1	1.2302 ± .0008	1.227 ± .00154	-.0032 ±.00173
	σ_2	1.6188 ± .0024	1.612 ± .0064	-.0068 ±.0068
	σ_3	25.644 ± .152	24.63 ± .387	-1.014 ±.419
	σ_4	387.09 ± 1.25	386.6 ± 2.98	-.49 ±3.25
U238 Absorption	σ_1	.43333 ± .00163	.4295 ± .00292	-.00383 ±.00334
	σ_2	.2422 ± .00097	.2427 ± .0060	.0005 ±.0061
	σ_3	2.0842 ± .0174	2.075 ± .0504	-.0092 ±.0533
	σ_4	1.8959 ± .0060	1.894 ± .0597	-.0019 ±.0600
U238 Fission	σ_1	.37870 ± .00171	.3746 ± .0035	-.0041 ±.0039
	σ_2	4.56-4 ± .032-4	4.55-4 ± .12-4	-.01-4 ±.124-4
	σ_3	2.6303-5 ± .339-5	2.33-5 ± 1.03-5	-.3-5 ±1.08-5
	σ_4	--	--	--

Figure 1 - k_{eff} vs Rho 28 for TRX-1 Full Core



The agreement is a result of interest. We have given a direct comparison of group cross sections obtained from cell and full core calculations and have found the two sets to be fully consistent.

In conclusion, it can be stated that the value of SAM-CE for reactor calculations has been demonstrated and valuable data has been obtained for testing the accuracy of ENDF/B-IV and ENDF/B-V libraries for reactor calculations.

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